K-Alpha Emission Spectra From Non-Equilibrium Ionizing Plasmas

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Abstract. Kα X-ray emission spectra from highly charged Fe ions have been theoretically predicted using a detailed and systematic spectral model. Account has been taken of the fundamental atomic radiative-emission processes associated with inner-shell electron collisional excitation and ionization, as well as dielectronic recombination. Particular emphasis has been directed at extreme non-equilibrium or transient-ionization conditions, which can occur in astrophysical and tokamak plasmas. Good agreement has been found in comparisons with spectral observations on the EBIT-II electron beam ion trap at the Lawrence Livermore National Laboratory. We have identified spectral features that can serve as diagnostics of the electron density, the line-formation mechanism, and the charge-state distribution.

Keywords: Autoionization, Radiative transitions, Inner-shell-electron collisional excitation and ionization, X-ray spectra, Equilibrium and non-equilibrium plasmas, Electron-ion interactions.
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I. INTRODUCTION

Kα emissions associated with 2p $\rightarrow$ 1s inner-shell-electron radiative transitions in highly ionized Fe ions occur as prominent satellite-line features in the X-ray spectra of laboratory and astrophysical plasmas. We have developed a detailed atomic spectral model [1] for the Kα radiative emissions produced by the iron ions from Fe XVIII to Fe XXIV, which occur in the spectral range from 1.84 Å to 1.94 Å. From an analysis of the Kα emission spectra, basic physical properties within the emitting region can be deduced, including temperatures, densities, charge-state populations, and electric- and magnetic-field distributions. In the development of spectral models for atomic radiative emissions in plasmas, the plasma electrons have been traditionally represented by a Maxwellian electron velocity (or energy) distribution function. In previous applications [1, 2] of our detailed atomic-physics model, computer simulations have been carried out for low-density (solar-corona), intermediate-density (tokamak), and high-density (laser-produced) plasmas using Maxwellian electron

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energy distributions. In this investigation, we present new results obtained from an extension of our previously reported investigations, in which an arbitrary electron energy distribution can be accommodated. This extension is necessary for the computer simulation of the Kα radiative emission from extreme non-equilibrium or transient-ionization environments.

II. ELEMENTARY RADIATIVE TRANSITIONS

Elementary transitions involving autoionizing resonances of multiply-charged ions are known to play important roles in the determination of the atomic-level population densities and charged-state distributions [3]. Radiative transitions from autoionizing states appear in the emission spectra as distinctive satellite features [4], in close proximity to a resonance line of the ion with one additional electron removed, e. g., the recombining ion in the two-step dielectronic recombination processes described by Burgess [5]. The spectral features produced by radiative transitions from autoionizing states may be observable as distinct spectroscopically resolvable satellite lines, as unresolvable enhancements of the associated resonance line, or as blends consisting of many overlapping satellite lines. For the precise computer simulation of the high-resolution Kα emission spectra, it is necessary to take into account the separate contributions from the individual fine-structure components of the 2p → 1s inner-shell-electron radiative transitions. Accordingly, the states involved in these radiative transitions must be specified in complete detail, as individual fine-structure states (hyperfine structure will be ignored). The autoionizing states of interest may be described as being approximately associated with the electronic configurations $1s^1 2s^r 2p^s$ (with $0 \leq r \leq 2$ and $0 \leq s \leq 6$) in the irons ions from Fe XVIII to Fe XXIV, with the understanding that these identifications cannot have a rigorous meaning within the framework of a fully-relativistic multi-configuration representation for the many-electron atomic states.

III. EXCITATION OF AUTOIONIZING STATES IN PLASMAS

In high-temperature plasmas, the autoionizing states can be populated by the radiationless electron-capture process, which is the first step in the two-step dielectronic recombination process. This indirect process is usually the dominant recombination mechanism for multiply-charged ions at low densities. In low-density plasmas, the initial ions undergoing radiationless electron capture can be assumed to be predominantly in their ground states (or perhaps in a metastable state). However, the dominant autoionization process may correspond to a transition leading to the formation of an excited state of the residual ion [6]. In addition, autoionization into excited states following radiationless electron capture can provide an important indirect (resonant) contribution to the total rate of electron impact excitation [7].

While radiationless electron capture is often the dominant excitation mechanism for the Kα emission in a high-temperature plasma, which is then commonly referred to as dielectronic-recombination satellite emission, it is also necessary to take into account the population of the autoionizing states as a result of the inner-shell-electron electron-impact excitation process. In addition, autoionization (instead of radiative decay) following inner-shell-electron excitation can provide an appreciable indirect (resonant) contribution to the total rate for electron impact ionization [8].

In the development of our earlier atomic spectral model [1] for the Kα emission of highly-charged Fe ions, we considered only radiationless electron capture and inner-shell-electron collisional excitation. In the present investigation, we have taken into account the additional population of the autoionizing states due to inner-shell-electron electron-impact ionization. Radiationless electron capture is expected to play the dominant role in plasmas under conditions near a steady-state ionization-recombination balance, e. g., as described by the low-density corona-model approximation discussed by Griem [9]. However, inner-shell-electron collisional excitation and ionization can provide the dominant Kα line-formation mechanism for extreme non-equilibrium, transient-ionization environments.

IV. SPECTRAL MODEL FOR NON-EQUILIBRIUM PLASMAS

In spectral models for atomic radiative emissions following electron-ion collisions in plasmas, the electron velocity distribution has been traditionally represented by a local-thermodynamic-equilibrium (Maxwellian) distribution function. The radiative emission spectra can then be predicted as functions of the local electron temperature. We have employed a natural extension of the traditional description, in which account can be taken of an arbitrary single-electron velocity (or energy) distribution function. Our investigation of the emission spectra produced by extreme non-equilibrium electron energy distributions has been carried out by means of computer simulations of the Fe Kα emission spectra observed from the EBIT-II electron beam ion trap facility at the Lawrence Livermore National Laboratory [10, 11]. Since the electron beam in EBIT-II is nearly mono-energetic, a precise investigation of the various fundamental Kα radiative emission processes can be carried out. In order to observe the contributions from the dielectronic recombination satellites, which are produced by radiationless electron capture, it had been necessary either to select the electron-beam energy at a particular resonance energy [12] or to vary the electron-beam energy in a continuous manner through the resonance region [13]. In the present investigation, Fe Kα radiative emission spectra have been theoretically predicted for two different non-resonant electron-beam energies, for which high-resolution spectra have been observed from EBIT-II [14]. These non-resonant energies, for which the dielectronic recombination process does not contribute, occur above and below the K-shell ionization threshold. From the comparison between the observed high-resolution Fe Kα radiative emission spectra [14] and the corresponding theoretically predicted spectra, the contributions from inner-shell-electron collisional excitation and ionization have been separately investigated, and the sensitivities of various Kα radiative emission lines to density variations and transient ionization conditions have been assessed.

V. DENSITY DEPENDENCE OF THE EMISSION SPECTRA

The decomposition of the Kα emission spectra into separate contributions associated with the three fundamental electron-ion collision processes cannot be made in an unambiguous manner and is strictly applicable only for low densities, for which the simple corona-model approximation is valid. With increasing electron density, the population densities of the radiating autoionizing states can be altered as a result of electron collisional transitions among the low-lying bound fine-structure states. A complete density-dependent description of the radiative emission spectra can be provided only on the basis of a detailed (possibly time-dependent) collisional-radiative model. In a systematic collisional-radiative model, the population densities of both the bound and autoionizing states would be self-consistently determined, taking into account the multitude of elementary collisional and radiative transitions together with the relevant autoionization processes.

In order to provide an approximate description of the density dependence of the Kα emission spectra, which would circumvent the need to consider the enormous collisional-radiative matrices corresponding to the multitude of the relevant fine-structure states, we have introduced a hierarchy of simple statistical models [1] for the distribution of the population of the initial ions among the various low-lying (bound) fine-structure states. At low densities, the initial-ion population can be assumed to be confined entirely to the lowest-lying fine-structure states of the ground-state electronic configurations. An approximate description of the population distribution for the moderate densities characteristic of tokamak plasmas, which is believed to be appropriate for the intermediate-density regime $10^{12} \leq N_e \leq 10^{14}$ cm^{-3}, can be provided by assuming that the collisional transitions are capable of establishing a statistical-equilibrium distribution of the initial-ion population among all fine-structure states belonging to the ground-state electronic configuration. At higher densities, which are encountered in laser-produced plasmas, we have assumed that a statistical-equilibrium distribution can be established between all fine-structure states of the ground-state and certain low-lying excited-state electronic configurations [1]. The collisional transitions among the autoionizing states, which can lead to strong density variations in dense laser-produced plasmas [15-17], have not been taken into account in our Kα spectral simulations.

VI. SPECTRAL SIMULATIONS

Employing the decomposition of the total Kα spectral intensity into the separate contributions associated with the three fundamental electron-ion collisional interactions, we have evaluated the individual radiative emission coefficients for the nearly mono-energetic electron beam of the EBIT-II experiment. In the low-density regime, the spectral line-shape functions are determined by Doppler broadening and by the broadening due to the permissible autoionization and spontaneous radiative emission processes. The initial Fe ions are assumed to be either in the ground fine-structure state or statistically distributed among all fine-structure states belonging to the ground-state electronic configuration. We have determined the charge-state distributions of the radiating atomic ions for both equilibrium and non-equilibrium environments. While the charge-state distributions in low-density high-temperature equilibrium plasmas are determined predominately by the (possibly dynamical) balance between electron-impact ionization (including autoionization following inner-shell-electron excitation) and direct radiative together with dielectronic recombination, a different physical situation is usually encountered in the description of the charge-state balance in extreme non-equilibrium or transient-ionization plasmas. An even more substantial departure from the familiar corona-equilibrium charge-state distributions can be produced in photoionized plasmas, for which radiative excitation, photoionization, and charge-transfer processes can play a significant role in the population of the autoionizing states. In the creation of sufficiently deep inner-shell-electron vacancies in heavy atomic ions, spontaneous decay can occur through a complex cascade process involving a sequence of radiative, Auger, and Coster Kronig transitions, which can result in a state of multiple ionization [18].

$K\alpha$ spectral simulations have been carried out for both equilibrium and non-equilibrium conditions [19]. To obtain spectral predictions that can be compared with the observed EBIT-II spectra, it has been necessary to include corrections to the theoretically predicted wavelengths. The wavelength corrections are in part due to an inadequate description in the atomic structure of the electron-electron correlations but are primarily attributable to the radiative corrections of quantum electrodynamics. In order to obtain agreement with the experimental spectra obtained from EBIT-II, the effects of electron density cannot be neglected. We have investigated the contributions of the various fundamental excitation processes under equilibrium and non-equilibrium conditions, and we have identified spectral features that are sensitive to density variations and to extreme non-equilibrium, transient-ionization conditions.

VII. FUTURE EXTENSIONS

In future extensions of this investigation, it would be desirable to include spectral contributions from more highly excited autoionizing states, which may blend with the features already included or produce new features. To provide a detailed determination of the populations of the fine-structure states, as functions of density, a systematic and self-consistent collisional-radiative model [3] should be developed. The ionization and recombination rate coefficients evaluated in this investigation are the low-density (corona-model) limits of effective transition rates, which are most rigorously introduced as a result of a reduced kinetic-theory description [3, 20] of the multitude of atomic collisional and radiative interactions. It will also be desirable to implement a more detailed description of the radiative emission processes [21], taking into account the angular distribution and polarization of the emitted photons that can be produced by directed-electron excitation. To obtain theoretical predictions beyond the isolated-resonance approximate, it is necessary to include quantum-mechanical interference effects, which have been investigated for radiative and dielectronic recombination [22, 23]. With increasing spectral resolution of the satellite observations, it may also be necessary to employ more sophisticated descriptions of the spectral line shapes, e. g., beyond the lowest-order approximation of QED perturbation theory. Using a densitymatrix approach [24], a self-consistent treatment can be provided for the atomic-population kinetics and the spectral-line shapes.

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